Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:37 PM GMT

PDB ID	:	1XSI
Title	:	Structure of a Family 31 alpha glycosidase
Authors	:	Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.
Deposited on	:	2004-10-19
Resolution	:	2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

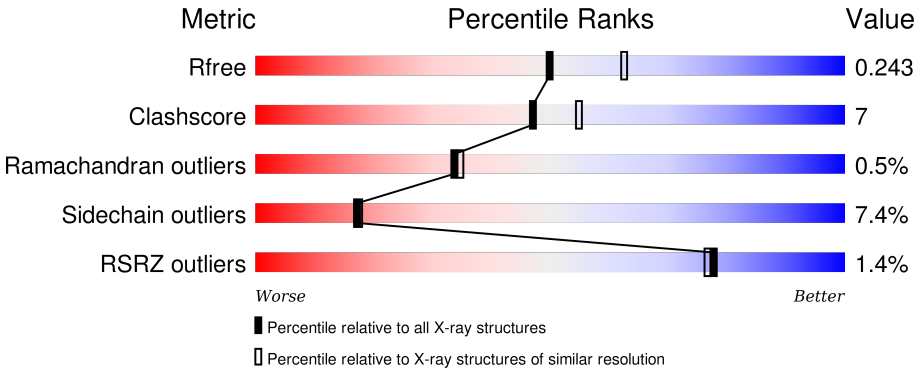
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	778	81% 15%
1	B	778	3% 77% 19%
1	C	778	80% 15%
1	D	778	2% 77% 19%
1	E	778	76% 20%

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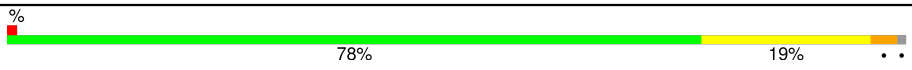
Mol	Chain	Length	Quality of chain
1	F	778	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	3016	-	-	-	X
2	SO4	C	3012	-	-	-	X
2	SO4	F	3009	-	-	X	-
4	ACY	A	2003	-	-	-	X
4	ACY	E	2001	-	-	-	X
4	ACY	F	2002	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38490 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	B	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	C	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	D	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	E	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	F	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	EXPRESSION TAG	UNP P31434
A	774	HIS	-	EXPRESSION TAG	UNP P31434
A	775	HIS	-	EXPRESSION TAG	UNP P31434
A	776	HIS	-	EXPRESSION TAG	UNP P31434
A	777	HIS	-	EXPRESSION TAG	UNP P31434
A	778	HIS	-	EXPRESSION TAG	UNP P31434
B	773	HIS	-	EXPRESSION TAG	UNP P31434
B	774	HIS	-	EXPRESSION TAG	UNP P31434
B	775	HIS	-	EXPRESSION TAG	UNP P31434
B	776	HIS	-	EXPRESSION TAG	UNP P31434
B	777	HIS	-	EXPRESSION TAG	UNP P31434
B	778	HIS	-	EXPRESSION TAG	UNP P31434
C	773	HIS	-	EXPRESSION TAG	UNP P31434
C	774	HIS	-	EXPRESSION TAG	UNP P31434
C	775	HIS	-	EXPRESSION TAG	UNP P31434
C	776	HIS	-	EXPRESSION TAG	UNP P31434
C	777	HIS	-	EXPRESSION TAG	UNP P31434

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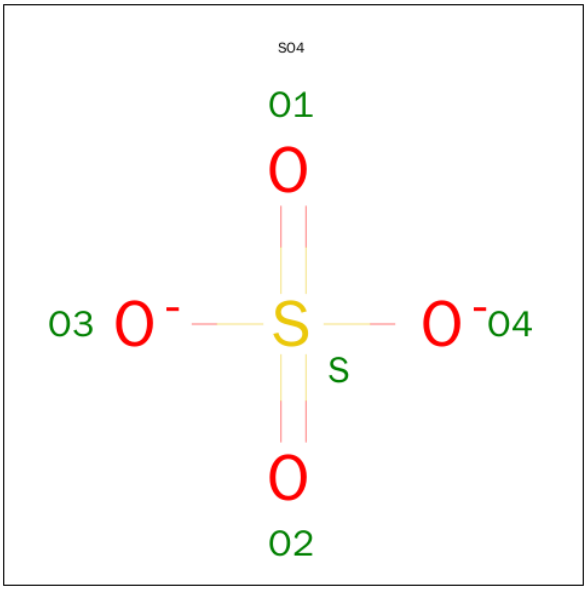
Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	EXPRESSION TAG	UNP P31434
D	773	HIS	-	EXPRESSION TAG	UNP P31434
D	774	HIS	-	EXPRESSION TAG	UNP P31434
D	775	HIS	-	EXPRESSION TAG	UNP P31434
D	776	HIS	-	EXPRESSION TAG	UNP P31434
D	777	HIS	-	EXPRESSION TAG	UNP P31434
D	778	HIS	-	EXPRESSION TAG	UNP P31434
E	773	HIS	-	EXPRESSION TAG	UNP P31434
E	774	HIS	-	EXPRESSION TAG	UNP P31434
E	775	HIS	-	EXPRESSION TAG	UNP P31434
E	776	HIS	-	EXPRESSION TAG	UNP P31434
E	777	HIS	-	EXPRESSION TAG	UNP P31434
E	778	HIS	-	EXPRESSION TAG	UNP P31434
F	773	HIS	-	EXPRESSION TAG	UNP P31434
F	774	HIS	-	EXPRESSION TAG	UNP P31434
F	775	HIS	-	EXPRESSION TAG	UNP P31434
F	776	HIS	-	EXPRESSION TAG	UNP P31434
F	777	HIS	-	EXPRESSION TAG	UNP P31434
F	778	HIS	-	EXPRESSION TAG	UNP P31434

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0

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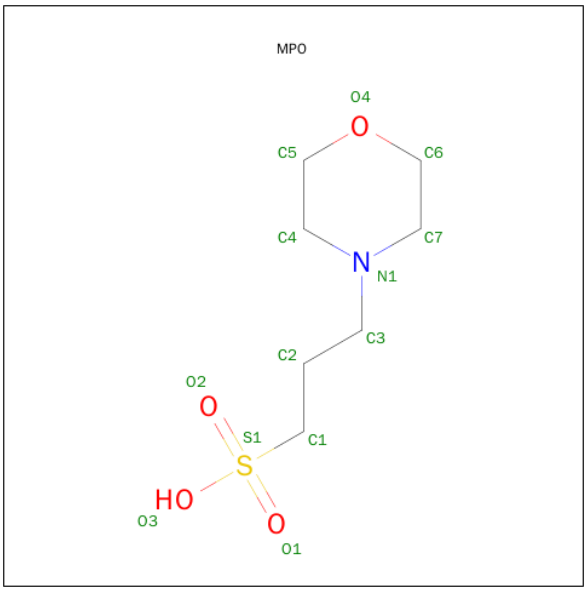
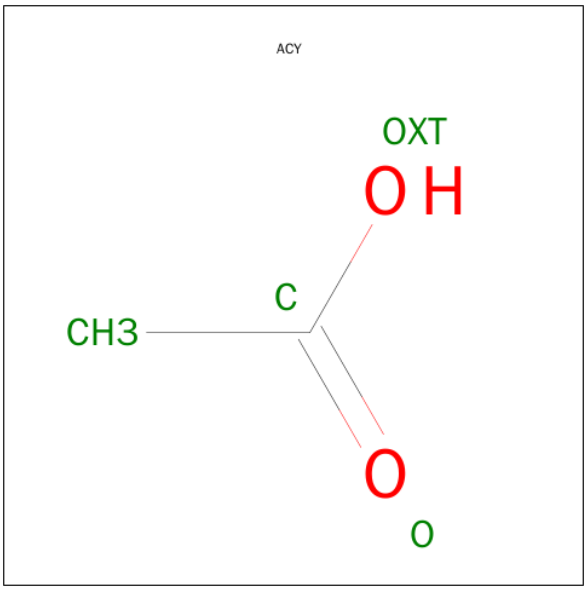
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
3	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

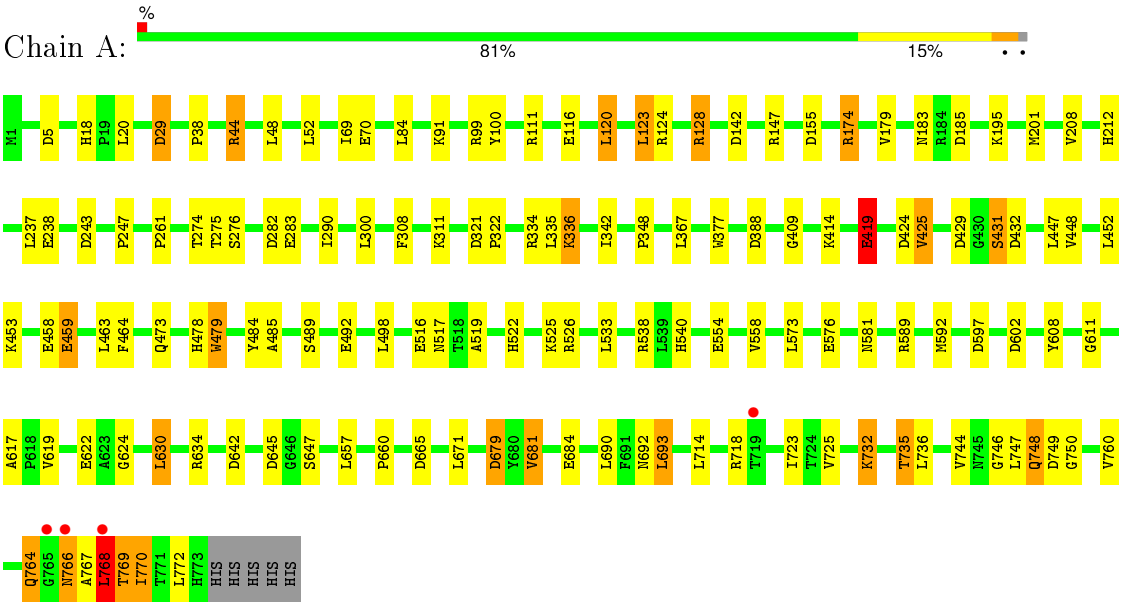
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	170	Total O 170 170	0	0
5	B	140	Total O 140 140	0	0
5	C	189	Total O 189 189	0	0
5	D	162	Total O 162 162	0	0
5	E	152	Total O 152 152	0	0
5	F	167	Total O 167 167	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

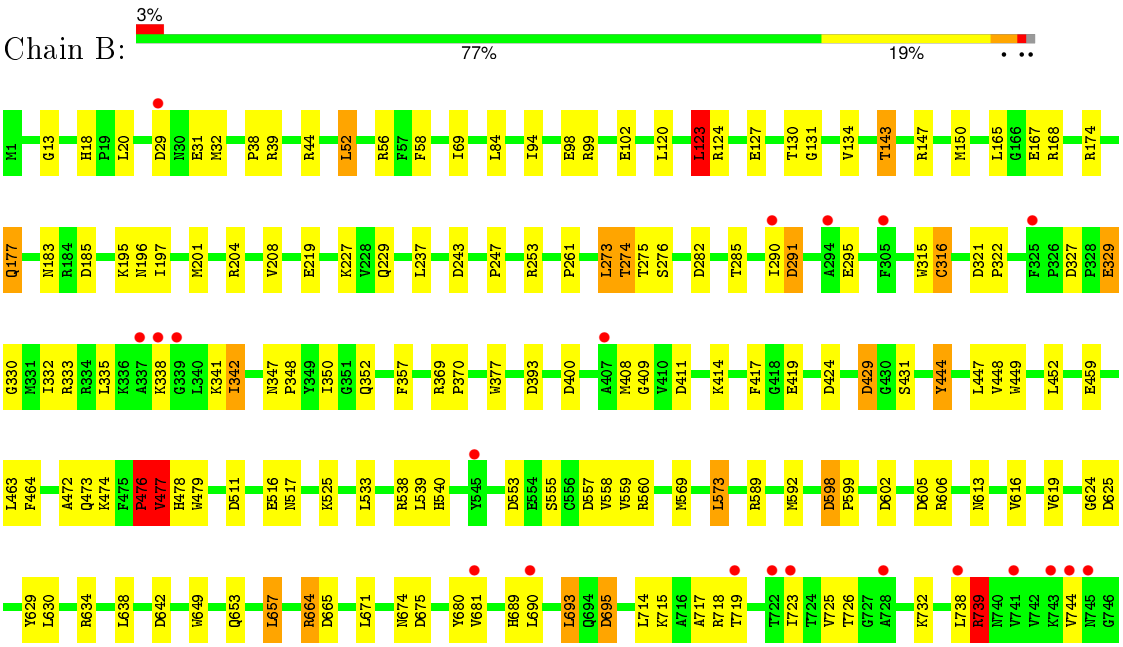
- Molecule 1: Putative family 31 glucosidase yicI

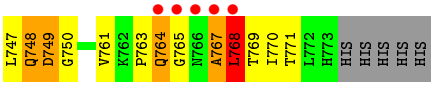
Chain A:



- Molecule 1: Putative family 31 glucosidase yicI

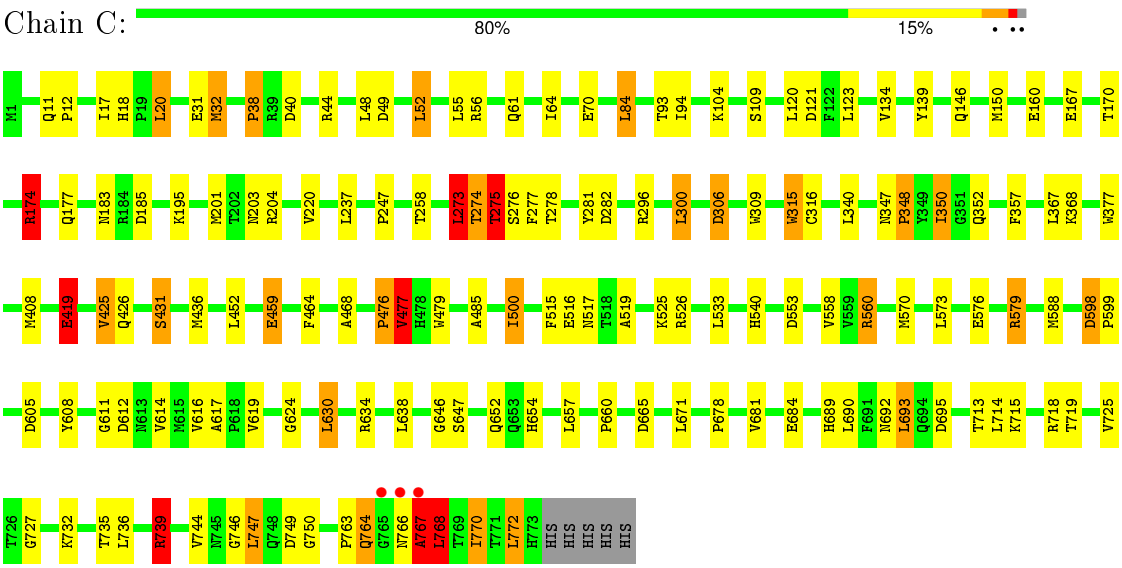
Chain B:





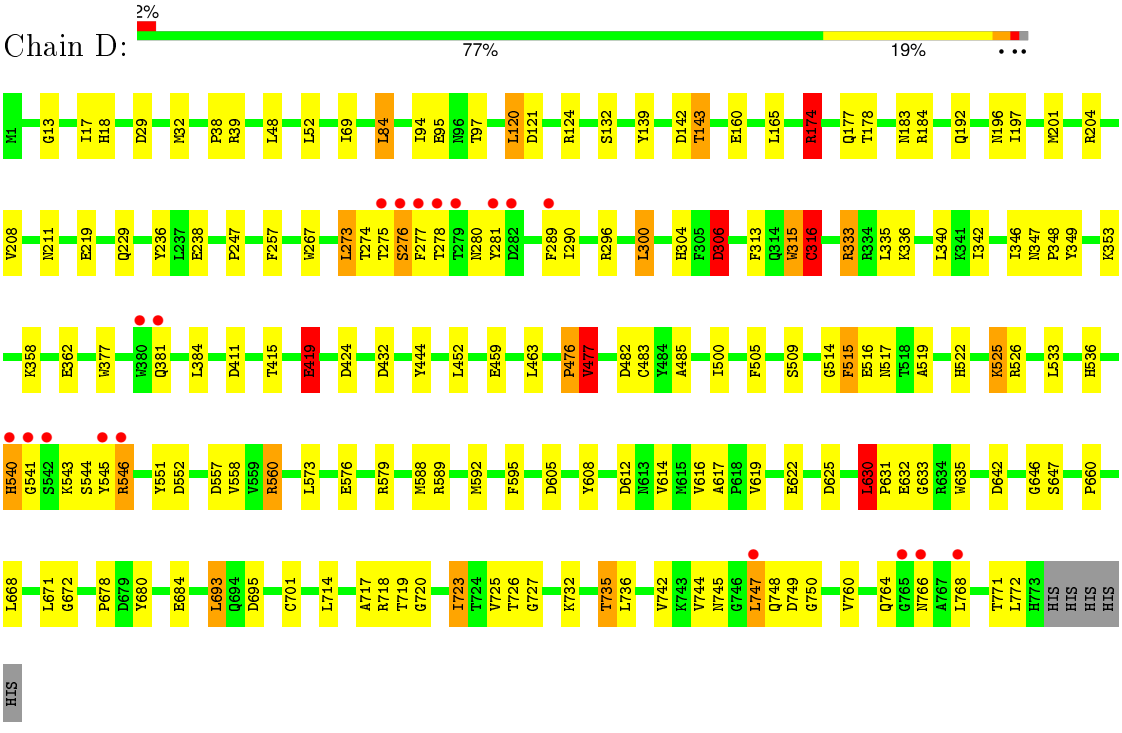
• Molecule 1: Putative family 31 glucosidase yicI

Chain C:



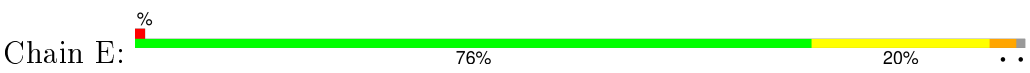
• Molecule 1: Putative family 31 glucosidase yicI

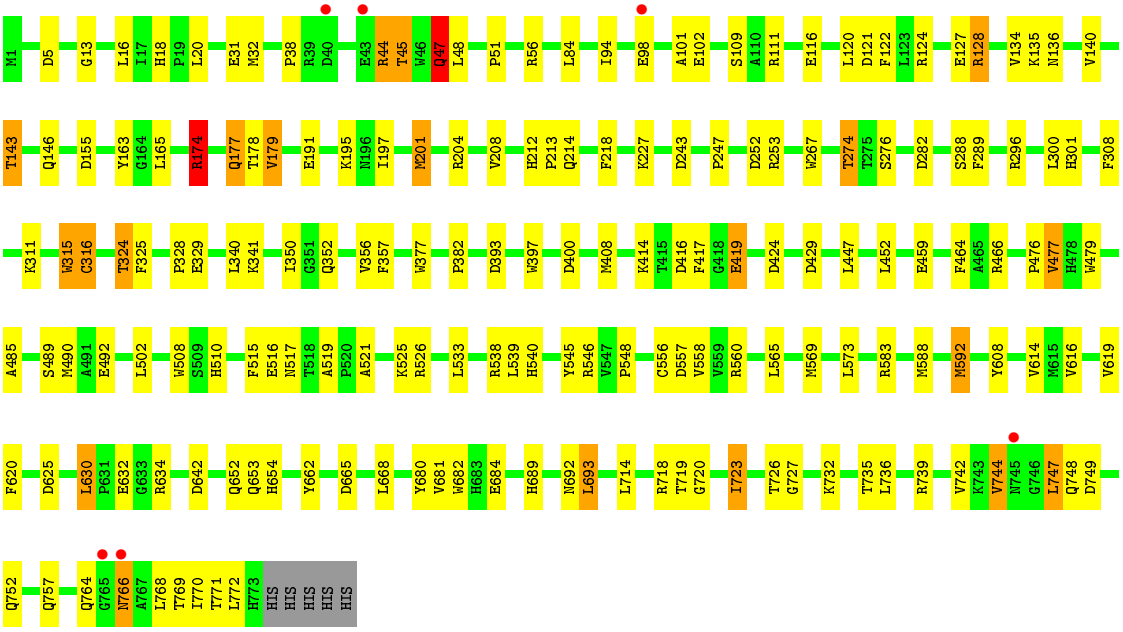
Chain D:



• Molecule 1: Putative family 31 glucosidase yicI

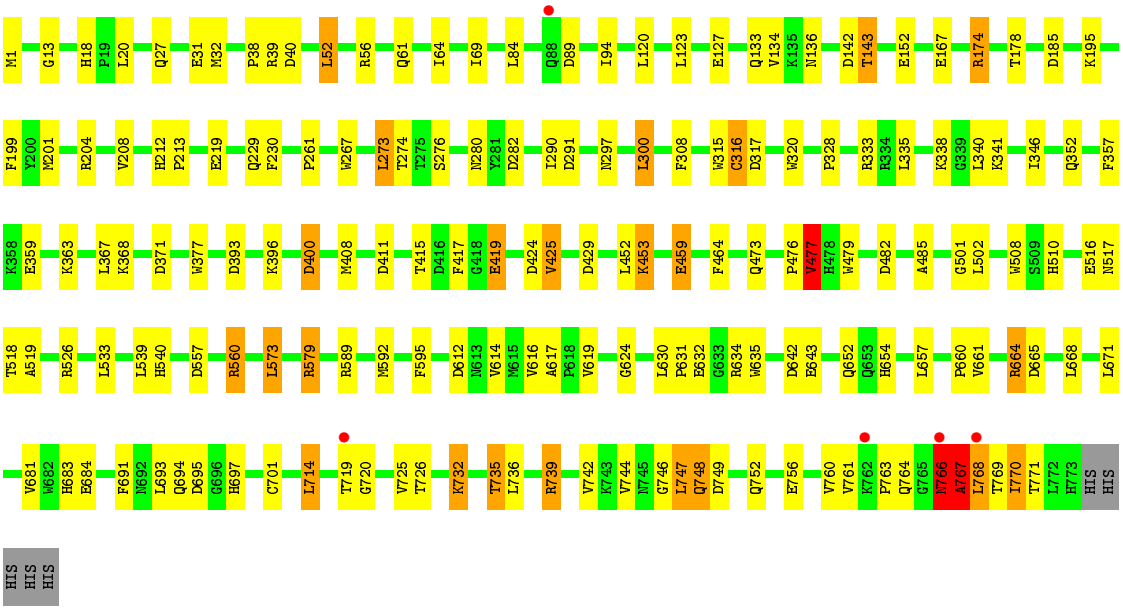
Chain E:





• Molecule 1: Putative family 31 glucosidase yicI

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	161.69Å 174.93Å 209.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 103.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.20) 98.8 (103.30-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.239 0.208 , 0.243	Depositor DCC
R_{free} test set	14932 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.714	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 30.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 295701 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	38490	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPO, ACY, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.90	0/6409	0.96	21/8711 (0.2%)
1	B	0.87	1/6409 (0.0%)	0.96	32/8711 (0.4%)
1	C	0.90	2/6409 (0.0%)	1.01	32/8711 (0.4%)
1	D	0.90	3/6409 (0.0%)	1.00	26/8711 (0.3%)
1	E	0.87	0/6409	0.95	20/8711 (0.2%)
1	F	0.95	2/6409 (0.0%)	1.00	35/8711 (0.4%)
All	All	0.90	8/38454 (0.0%)	0.98	166/52266 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	1
1	C	2	1
1	D	1	2
1	E	2	1
1	F	2	0
All	All	8	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	306	ASP	CB-CG	9.89	1.72	1.51
1	C	32	MET	SD-CE	-5.94	1.44	1.77
1	F	661	VAL	CB-CG1	5.93	1.65	1.52
1	D	236	TYR	CD1-CE1	5.68	1.47	1.39
1	C	431	SER	CB-OG	-5.58	1.34	1.42
1	D	306	ASP	CA-CB	5.11	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	444	TYR	CE2-CZ	5.07	1.45	1.38
1	F	691	PHE	CE1-CZ	5.05	1.47	1.37

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	306	ASP	CB-CG-OD1	12.92	129.93	118.30
1	C	560	ARG	NE-CZ-NH1	-12.14	114.23	120.30
1	D	174	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	E	174	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	C	174	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	C	174	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	F	739	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	C	739	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	C	665	ASP	CB-CG-OD2	8.51	125.96	118.30
1	D	29	ASP	CB-CG-OD2	8.48	125.93	118.30
1	D	174	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	174	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	F	560	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	589	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	F	174	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	511	ASP	CB-CG-OD2	8.10	125.59	118.30
1	F	476	PRO	CA-C-N	-8.09	99.40	117.20
1	E	476	PRO	CA-C-N	-8.01	99.58	117.20
1	E	174	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	400	ASP	CB-CG-OD2	7.99	125.49	118.30
1	B	29	ASP	CB-CG-OD2	7.87	125.38	118.30
1	B	560	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	D	560	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	F	482	ASP	CB-CG-OD2	7.50	125.05	118.30
1	E	424	ASP	CB-CG-OD2	7.48	125.03	118.30
1	C	749	ASP	CB-CG-OD2	7.42	124.98	118.30
1	F	174	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	F	560	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	F	665	ASP	CB-CG-OD2	7.35	124.92	118.30
1	D	306	ASP	OD1-CG-OD2	-7.31	109.41	123.30
1	A	665	ASP	CB-CG-OD2	7.28	124.86	118.30
1	F	612	ASP	CB-CG-OD1	7.27	124.84	118.30
1	C	476	PRO	C-N-CA	7.17	139.64	121.70
1	B	665	ASP	CB-CG-OD2	7.06	124.66	118.30
1	C	739	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	147	ARG	NE-CZ-NH1	-6.92	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	121	ASP	CB-CG-OD2	6.91	124.52	118.30
1	E	665	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	282	ASP	CB-CG-OD2	6.85	124.46	118.30
1	E	429	ASP	CB-CG-OD2	6.83	124.44	118.30
1	C	315	TRP	C-N-CA	6.82	138.74	121.70
1	E	476	PRO	C-N-CA	6.82	138.74	121.70
1	B	477	VAL	CB-CA-C	6.81	124.34	111.40
1	C	282	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	174	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	F	476	PRO	C-N-CA	6.71	138.48	121.70
1	B	316	CYS	CA-CB-SG	-6.70	101.95	114.00
1	C	612	ASP	CB-CG-OD2	6.69	124.32	118.30
1	E	5	ASP	CB-CG-OD2	6.69	124.32	118.30
1	A	424	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	560	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	E	201	MET	CG-SD-CE	-6.67	89.52	100.20
1	C	476	PRO	CA-C-N	-6.62	102.64	117.20
1	D	411	ASP	CB-CG-OD2	6.58	124.22	118.30
1	F	573	LEU	CB-CG-CD1	6.56	122.16	111.00
1	B	123	LEU	CA-CB-CG	6.54	130.35	115.30
1	F	477	VAL	CB-CA-C	6.54	123.83	111.40
1	C	185	ASP	CB-CG-OD2	6.51	124.16	118.30
1	F	52	LEU	CA-CB-CG	6.46	130.16	115.30
1	C	49	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	695	ASP	CB-CG-OD2	6.38	124.04	118.30
1	E	121	ASP	CB-CG-OD2	6.36	124.02	118.30
1	F	429	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	419	GLU	CA-CB-CG	6.33	127.32	113.40
1	F	739	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	476	PRO	CA-C-N	-6.26	103.42	117.20
1	B	253	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	F	371	ASP	CB-CG-OD2	6.13	123.82	118.30
1	D	476	PRO	C-N-CA	6.12	137.00	121.70
1	F	739	ARG	CG-CD-NE	-6.11	98.97	111.80
1	E	315	TRP	C-N-CA	6.10	136.96	121.70
1	C	425	VAL	CG1-CB-CG2	-6.08	101.18	110.90
1	C	477	VAL	CB-CA-C	6.08	122.94	111.40
1	D	316	CYS	CA-CB-SG	-6.06	103.08	114.00
1	F	315	TRP	CA-C-N	-6.06	103.87	117.20
1	B	52	LEU	CA-CB-CG	6.02	129.15	115.30
1	D	612	ASP	CB-CG-OD1	6.02	123.72	118.30
1	F	642	ASP	CB-CG-OD2	5.98	123.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	317	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	393	ASP	CB-CG-OD2	5.94	123.65	118.30
1	D	316	CYS	N-CA-C	5.89	126.91	111.00
1	B	411	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	273	LEU	CB-CG-CD2	5.87	120.97	111.00
1	D	419	GLU	CA-CB-CG	5.86	126.28	113.40
1	A	29	ASP	CB-CG-OD2	5.85	123.57	118.30
1	F	767	ALA	N-CA-C	-5.84	95.23	111.00
1	F	185	ASP	CB-CG-OD2	5.83	123.55	118.30
1	E	642	ASP	CB-CG-OD2	5.83	123.54	118.30
1	B	424	ASP	CB-CG-OD2	5.83	123.54	118.30
1	E	393	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	274	THR	OG1-CB-CG2	-5.78	96.70	110.00
1	C	419	GLU	CA-CB-CG	5.77	126.09	113.40
1	A	282	ASP	CB-CG-OD2	5.75	123.47	118.30
1	D	142	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	602	ASP	CB-CG-OD2	5.73	123.45	118.30
1	B	642	ASP	CB-CG-OD2	5.72	123.44	118.30
1	F	411	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	739	ARG	CG-CD-NE	-5.70	99.83	111.80
1	E	316	CYS	N-CA-C	5.67	126.31	111.00
1	F	424	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	40	ASP	CB-CG-OD2	5.64	123.38	118.30
1	E	315	TRP	CA-C-N	-5.61	104.86	117.20
1	D	424	ASP	CB-CG-OD2	5.61	123.34	118.30
1	A	602	ASP	CB-CG-OD2	5.59	123.33	118.30
1	F	40	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	642	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	749	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	429	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	739	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	E	749	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	253	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	589	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	A	142	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	121	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	553	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	123	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	749	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	645	ASP	CB-CG-OD2	5.50	123.25	118.30
1	F	393	ASP	CB-CG-OD2	5.48	123.23	118.30
1	C	275	THR	N-CA-CB	-5.47	99.91	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	598	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	185	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	675	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	5	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	388	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	630	LEU	CB-CG-CD1	5.42	120.21	111.00
1	A	679	ASP	CB-CG-OD2	5.42	123.18	118.30
1	D	589	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	D	124	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	F	282	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	315	TRP	CA-C-N	-5.36	105.41	117.20
1	D	605	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	605	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	557	ASP	CB-CG-OD2	5.33	123.09	118.30
1	E	253	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	F	315	TRP	C-N-CA	5.33	135.02	121.70
1	F	142	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	52	LEU	CB-CG-CD2	5.31	120.03	111.00
1	D	477	VAL	N-CA-C	5.31	125.33	111.00
1	F	749	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	482	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	598	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	432	ASP	CB-CG-OD1	5.27	123.04	118.30
1	F	664	ARG	CB-CA-C	-5.26	99.88	110.40
1	B	476	PRO	CA-C-N	-5.26	105.64	117.20
1	E	282	ASP	CB-CG-OD2	5.25	123.03	118.30
1	F	400	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	597	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	477	VAL	N-CA-C	5.25	125.16	111.00
1	C	52	LEU	CA-CB-CG	5.24	127.36	115.30
1	F	89	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	630	LEU	CA-CB-CG	5.24	127.35	115.30
1	D	642	ASP	CB-CG-OD2	5.24	123.01	118.30
1	F	579	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	20	LEU	CA-CB-CG	5.20	127.26	115.30
1	F	695	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	605	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	739	ARG	CG-CD-NE	-5.14	101.00	111.80
1	B	291	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	147	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	120	LEU	CA-CB-CG	5.07	126.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	625	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	767	ALA	N-CA-C	-5.02	97.44	111.00
1	E	400	ASP	CB-CG-OD2	5.01	122.81	118.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	477	VAL	CA
1	C	316	CYS	CA
1	C	477	VAL	CA
1	D	477	VAL	CA
1	E	316	CYS	CA
1	E	477	VAL	CA
1	F	316	CYS	CA
1	F	477	VAL	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	766	ASN	Peptide
1	B	476	PRO	Peptide
1	C	476	PRO	Peptide
1	D	315	TRP	Peptide
1	D	476	PRO	Peptide
1	E	766	ASN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6226	0	5934	73	0
1	B	6226	0	5934	89	0
1	C	6226	0	5934	105	0
1	D	6226	0	5934	95	0
1	E	6226	0	5934	98	0
1	F	6226	0	5934	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	15	0	0	0	0
2	B	25	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	25	0	0	4	0
3	B	13	0	15	0	0
3	C	13	0	15	0	0
3	D	13	0	15	0	0
3	E	13	0	15	0	0
4	A	4	0	3	0	0
4	E	4	0	3	0	0
4	F	4	0	3	0	0
5	A	170	0	0	2	0
5	B	140	0	0	4	0
5	C	189	0	0	1	0
5	D	162	0	0	2	0
5	E	152	0	0	7	0
5	F	167	0	0	2	0
All	All	38490	0	35673	548	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (548) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:MET:HE2	1:C:94:ILE:HG23	1.20	1.19
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.23	1.17
1:F:274:THR:HG22	1:F:276:SER:H	0.98	1.10
1:B:274:THR:HG22	1:B:276:SER:H	1.13	1.10
1:E:274:THR:HG21	1:E:540:HIS:ND1	1.68	1.08
1:C:93:THR:HG22	1:C:104:LYS:HB3	1.36	1.07
1:B:274:THR:HG21	1:B:540:HIS:ND1	1.69	1.06
1:C:367:LEU:HD11	1:C:425:VAL:HG21	1.33	1.06
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.72	1.03
1:E:274:THR:HG22	1:E:276:SER:H	1.24	1.00
1:D:32:MET:HE2	1:D:94:ILE:HG23	1.44	0.99
1:D:32:MET:CE	1:D:94:ILE:HG23	1.95	0.96
1:F:735:THR:HG22	5:F:3174:HOH:O	1.66	0.94
1:F:274:THR:HG22	1:F:276:SER:N	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:HG22	1:A:276:SER:H	1.31	0.93
1:C:274:THR:HG21	1:C:540:HIS:ND1	1.84	0.93
1:D:381:GLN:HB2	1:D:384:LEU:HD12	1.50	0.93
1:C:274:THR:HG23	1:C:276:SER:H	1.36	0.91
1:A:274:THR:HG21	1:A:540:HIS:ND1	1.85	0.91
1:E:274:THR:CG2	1:E:276:SER:H	1.84	0.91
1:C:367:LEU:CD1	1:C:425:VAL:HG21	2.01	0.89
1:B:274:THR:CG2	1:B:276:SER:H	1.85	0.89
1:A:201:MET:HE1	1:A:247:PRO:HB3	1.54	0.88
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.57	0.86
1:D:13:GLY:O	1:D:143:THR:HB	1.74	0.86
1:A:770:ILE:HD11	1:A:772:LEU:HD23	1.59	0.85
1:D:540:HIS:CD2	1:D:541:GLY:N	2.45	0.84
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.60	0.84
1:C:32:MET:CE	1:C:94:ILE:HG23	2.04	0.82
1:B:274:THR:HG22	1:B:276:SER:N	1.94	0.82
1:F:290:ILE:CD1	1:F:335:LEU:HD22	2.09	0.82
1:B:32:MET:CE	1:B:94:ILE:HG23	2.07	0.82
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.11	0.81
1:C:368:LYS:O	1:C:425:VAL:HG23	1.83	0.79
1:A:274:THR:HG22	1:A:276:SER:N	1.97	0.79
1:C:638:LEU:O	1:C:739:ARG:NH2	2.15	0.79
1:A:525:LYS:HG2	1:A:558:VAL:HG21	1.63	0.78
1:D:727:GLY:H	1:D:766:ASN:HD21	1.31	0.78
1:C:274:THR:CG2	1:C:540:HIS:HA	2.13	0.78
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.66	0.78
1:C:425:VAL:HG22	1:C:426:GLN:N	1.96	0.77
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.66	0.77
1:C:93:THR:CG2	1:C:104:LYS:HB3	2.12	0.77
1:F:274:THR:CG2	1:F:276:SER:H	1.91	0.77
1:F:13:GLY:O	1:F:143:THR:HB	1.84	0.76
1:B:695:ASP:HA	1:B:718:ARG:HG2	1.68	0.76
1:E:13:GLY:O	1:E:143:THR:HB	1.86	0.76
1:B:332:ILE:HD12	1:B:333:ARG:N	2.01	0.75
1:C:425:VAL:CG2	1:C:426:GLN:N	2.49	0.75
1:C:274:THR:HG21	1:C:540:HIS:HA	1.69	0.75
1:C:367:LEU:HD11	1:C:425:VAL:CG2	2.16	0.75
1:B:761:VAL:HG11	1:B:768:LEU:HD21	1.68	0.74
1:C:32:MET:HE2	1:C:94:ILE:CG2	2.11	0.73
1:D:735:THR:HG23	1:D:760:VAL:HG13	1.70	0.73
2:E:3006:SO4:O2	5:E:3083:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:ILE:HD11	1:C:772:LEU:HD13	1.73	0.71
1:D:315:TRP:HE3	1:D:381:GLN:CD	1.94	0.71
1:E:744:VAL:HG21	1:E:770:ILE:HG22	1.71	0.71
1:A:767:ALA:O	1:A:769:THR:N	2.24	0.71
1:B:638:LEU:O	1:B:739:ARG:NH2	2.23	0.70
1:A:212:HIS:HE1	1:A:238:GLU:H	1.39	0.70
1:A:290:ILE:HD13	1:A:335:LEU:HD22	1.73	0.70
1:A:735:THR:HG23	1:A:760:VAL:HG13	1.74	0.70
1:D:275:THR:O	1:D:276:SER:HB2	1.91	0.69
1:A:212:HIS:CE1	1:A:238:GLU:H	2.10	0.69
1:A:128:ARG:NH1	1:A:155:ASP:OD2	2.26	0.69
1:A:748:GLN:HG2	1:A:769:THR:HG23	1.74	0.69
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.73	0.69
1:C:275:THR:HG23	1:C:281:TYR:CE1	2.29	0.68
1:D:672:GLY:HA3	1:D:680:TYR:OH	1.93	0.68
1:F:201:MET:CE	1:F:502:LEU:HD23	2.24	0.68
1:D:315:TRP:CE3	1:D:381:GLN:NE2	2.62	0.68
1:C:525:LYS:HG2	1:C:558:VAL:HG21	1.75	0.68
1:E:165:LEU:HD13	1:E:179:VAL:HG11	1.75	0.68
1:E:38:PRO:HD3	1:E:51:PRO:O	1.93	0.68
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.75	0.67
1:D:540:HIS:CD2	1:D:540:HIS:C	2.68	0.67
1:E:179:VAL:HG13	1:E:218:PHE:HB2	1.77	0.66
1:F:681:VAL:HG12	2:F:3005:SO4:O3	1.95	0.66
1:E:324:THR:HG22	1:E:325:PHE:CD2	2.29	0.66
1:E:274:THR:HG22	1:E:276:SER:N	2.04	0.66
1:E:668:LEU:HD21	1:E:714:LEU:HD23	1.78	0.66
1:D:333:ARG:HH11	1:D:333:ARG:HG3	1.59	0.66
1:D:39:ARG:HD2	5:D:3063:HOH:O	1.96	0.66
1:E:356:VAL:HG11	1:E:397:TRP:HZ2	1.60	0.66
1:B:124:ARG:HD3	1:B:243:ASP:OD1	1.96	0.66
1:D:32:MET:HE2	1:D:94:ILE:CG2	2.21	0.65
1:E:32:MET:HE1	1:E:101:ALA:HB1	1.79	0.65
1:C:275:THR:HG22	1:C:276:SER:O	1.97	0.65
1:B:13:GLY:O	1:B:143:THR:HB	1.97	0.65
1:D:315:TRP:CE3	1:D:381:GLN:CD	2.71	0.64
1:E:300:LEU:HD12	1:E:340:LEU:HD21	1.79	0.64
1:E:592:MET:HE2	5:E:3145:HOH:O	1.98	0.64
1:D:274:THR:HG23	1:D:304:HIS:HD2	1.63	0.63
1:E:684:GLU:HG2	1:E:732:LYS:HB2	1.79	0.63
1:D:300:LEU:HD13	1:D:340:LEU:HD21	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:516:GLU:O	1:F:517:ASN:HB2	1.97	0.63
1:F:290:ILE:CD1	1:F:335:LEU:CD2	2.77	0.63
1:E:44:ARG:HA	1:E:47:GLN:HB2	1.80	0.63
1:E:356:VAL:HG11	1:E:397:TRP:CZ2	2.34	0.62
1:D:315:TRP:CZ3	1:D:381:GLN:NE2	2.66	0.62
1:D:201:MET:HE1	1:D:247:PRO:HB3	1.81	0.62
1:A:693:LEU:HD13	1:A:718:ARG:HB2	1.81	0.62
1:D:519:ALA:O	1:D:551:TYR:HE2	1.82	0.62
1:B:174:ARG:O	1:B:177:GLN:HG3	1.98	0.62
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.82	0.62
1:B:347:ASN:HB2	1:B:348:PRO:HD3	1.82	0.61
1:A:447:LEU:HD23	1:A:447:LEU:C	2.20	0.61
1:C:693:LEU:HD13	1:C:718:ARG:HB2	1.81	0.61
1:E:128:ARG:NH1	1:E:155:ASP:OD2	2.32	0.61
1:A:749:ASP:HB3	1:A:764:GLN:O	2.01	0.60
1:D:540:HIS:HA	1:D:546:ARG:HG3	1.83	0.60
1:A:770:ILE:HD11	1:A:772:LEU:CD2	2.29	0.60
1:F:747:LEU:HD12	1:F:752:GLN:HE21	1.67	0.60
1:B:39:ARG:HD2	5:B:3140:HOH:O	2.00	0.60
1:E:328:PRO:HD2	5:E:3147:HOH:O	2.02	0.60
1:A:212:HIS:CE1	1:A:237:LEU:HD12	2.37	0.60
1:E:662:TYR:OH	5:E:3121:HOH:O	2.16	0.59
1:E:592:MET:CE	5:E:3145:HOH:O	2.50	0.59
1:D:522:HIS:CG	1:D:622:GLU:HG3	2.38	0.59
1:F:735:THR:HG23	1:F:760:VAL:HG13	1.84	0.59
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.38	0.59
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.85	0.58
1:C:690:LEU:HD11	1:C:693:LEU:HG	1.84	0.58
1:E:693:LEU:HD13	1:E:718:ARG:HB2	1.85	0.58
1:D:290:ILE:HD13	1:D:335:LEU:HD22	1.85	0.58
1:F:290:ILE:HD13	1:F:335:LEU:HD22	1.83	0.58
1:A:485:ALA:HB1	1:A:519:ALA:HB2	1.86	0.58
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.85	0.58
1:C:274:THR:HG22	1:C:540:HIS:HA	1.83	0.58
1:D:274:THR:HG22	1:D:276:SER:H	1.68	0.58
1:A:290:ILE:HD13	1:A:335:LEU:CD2	2.33	0.57
1:F:20:LEU:HD22	1:F:134:VAL:CG2	2.34	0.57
1:A:767:ALA:C	1:A:769:THR:N	2.58	0.57
1:E:744:VAL:HG22	1:E:771:THR:O	2.03	0.57
1:B:689:HIS:ND1	1:B:739:ARG:NH1	2.52	0.57
1:E:533:LEU:HD21	1:E:569:MET:HE1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ASP:OD1	1:D:540:HIS:HE1	1.88	0.57
1:E:38:PRO:CD	1:E:51:PRO:O	2.52	0.57
1:E:652:GLN:NE2	5:E:3121:HOH:O	2.38	0.57
1:E:516:GLU:O	1:E:517:ASN:HB2	2.03	0.57
1:C:689:HIS:CE1	1:C:739:ARG:HH11	2.23	0.57
1:F:579:ARG:HG3	1:F:579:ARG:HH11	1.69	0.57
1:B:449:TRP:CH2	1:B:476:PRO:HD2	2.39	0.57
1:B:261:PRO:HA	1:B:473:GLN:O	2.05	0.56
1:A:212:HIS:HE1	1:A:237:LEU:HD12	1.69	0.56
1:E:565:LEU:HG	1:E:569:MET:CE	2.35	0.56
1:B:201:MET:CE	1:B:247:PRO:HB3	2.34	0.56
1:D:557:ASP:OD1	1:D:560:ARG:NH2	2.38	0.56
1:E:557:ASP:OD1	1:E:560:ARG:NH2	2.39	0.56
1:C:681:VAL:HG23	1:C:681:VAL:O	2.05	0.56
1:B:516:GLU:O	1:B:517:ASN:HB2	2.05	0.56
1:E:417:PHE:HA	1:E:419:GLU:OE2	2.05	0.56
1:F:557:ASP:OD1	1:F:560:ARG:NH2	2.39	0.56
1:B:201:MET:HE3	1:B:247:PRO:HB3	1.87	0.55
1:B:763:PRO:HB3	1:B:768:LEU:HD12	1.88	0.55
1:D:32:MET:HE1	1:D:94:ILE:HG23	1.82	0.55
1:F:133:GLN:HB2	1:F:136:ASN:HD22	1.71	0.55
1:D:735:THR:CG2	1:D:760:VAL:HG13	2.34	0.55
1:F:725:VAL:HB	1:F:768:LEU:HB3	1.87	0.55
1:D:296:ARG:O	1:D:560:ARG:NH1	2.38	0.55
1:A:429:ASP:OD1	1:A:431:SER:OG	2.24	0.55
1:C:183:ASN:HB3	1:C:419:GLU:HB3	1.87	0.54
1:B:569:MET:HB2	1:B:573:LEU:HD22	1.89	0.54
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.55	0.54
1:E:727:GLY:H	1:E:766:ASN:HD21	1.56	0.54
1:C:515:PHE:CD1	1:C:516:GLU:HG2	2.42	0.54
1:E:124:ARG:HD3	1:E:243:ASP:OD1	2.07	0.54
1:E:174:ARG:O	1:E:177:GLN:HG3	2.07	0.54
1:C:275:THR:HG23	1:C:281:TYR:CD1	2.43	0.54
1:E:485:ALA:HB1	1:E:519:ALA:HB2	1.89	0.54
1:A:183:ASN:HB3	1:A:419:GLU:HB3	1.88	0.54
1:F:681:VAL:CG2	1:F:683:HIS:CE1	2.91	0.54
1:B:332:ILE:HG12	1:B:408:MET:O	2.07	0.54
1:E:289:PHE:HZ	1:E:545:TYR:CD1	2.25	0.54
1:D:630:LEU:O	1:D:647:SER:N	2.39	0.54
1:A:617:ALA:O	1:A:660:PRO:HD2	2.08	0.54
1:C:747:LEU:HD13	1:C:750:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:THR:CG2	1:D:304:HIS:HD2	2.19	0.54
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.08	0.54
1:E:252:ASP:HA	1:E:583:ARG:O	2.07	0.54
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.89	0.54
1:A:44:ARG:HD2	1:F:308:PHE:CE1	2.42	0.54
1:D:727:GLY:N	1:D:766:ASN:HD21	2.04	0.54
1:F:508:TRP:CZ3	1:F:510:HIS:CD2	2.96	0.53
1:A:735:THR:CG2	1:A:760:VAL:HG13	2.39	0.53
1:D:525:LYS:NZ	1:D:552:ASP:OD2	2.40	0.53
1:A:336:LYS:HE2	1:A:409:GLY:O	2.08	0.53
1:C:274:THR:HG23	1:C:276:SER:N	2.14	0.53
1:E:747:LEU:HD12	1:E:752:GLN:NE2	2.23	0.53
1:E:634:ARG:HG2	1:E:692:ASN:ND2	2.23	0.53
1:A:516:GLU:O	1:A:517:ASN:HB2	2.08	0.53
1:E:414:LYS:NZ	1:E:538:ARG:HH12	2.07	0.53
1:F:595:PHE:CE1	1:F:631:PRO:HG2	2.44	0.53
1:A:283:GLU:OE1	1:A:334:ARG:NH1	2.41	0.53
1:C:367:LEU:CG	1:C:425:VAL:HG21	2.39	0.53
1:A:526:ARG:HD2	1:A:619:VAL:HB	1.90	0.53
1:E:274:THR:CG2	1:E:276:SER:N	2.66	0.53
1:B:750:GLY:HA2	1:B:764:GLN:HG2	1.91	0.53
1:C:296:ARG:O	1:C:560:ARG:NH1	2.32	0.53
1:E:329:GLU:HB2	1:E:408:MET:HG2	1.91	0.52
1:B:681:VAL:O	1:B:681:VAL:HG13	2.10	0.52
1:C:560:ARG:HH11	1:C:560:ARG:HG3	1.73	0.52
1:C:695:ASP:OD1	1:C:719:THR:O	2.27	0.52
1:D:617:ALA:O	1:D:660:PRO:HD2	2.10	0.52
1:A:767:ALA:C	1:A:769:THR:H	2.13	0.52
1:E:136:ASN:ND2	1:E:227:LYS:HE3	2.24	0.52
1:E:447:LEU:C	1:E:447:LEU:HD23	2.30	0.52
1:C:689:HIS:ND1	1:C:739:ARG:NH1	2.47	0.52
1:B:332:ILE:CD1	1:B:408:MET:O	2.57	0.52
1:B:748:GLN:HB2	1:B:769:THR:HB	1.92	0.52
1:E:521:ALA:O	1:E:525:LYS:HD3	2.10	0.52
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.45	0.52
1:C:347:ASN:HB2	1:C:348:PRO:CD	2.40	0.52
1:D:18:HIS:O	1:D:38:PRO:HA	2.09	0.52
1:E:102:GLU:HB2	1:E:111:ARG:HG3	1.91	0.52
1:D:632:GLU:HG3	1:D:633:GLY:N	2.26	0.52
1:B:767:ALA:O	1:B:768:LEU:C	2.48	0.51
1:E:565:LEU:HG	1:E:569:MET:HE2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:MET:CE	1:F:94:ILE:HG23	2.39	0.51
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.92	0.51
1:C:70:GLU:HG3	5:C:3103:HOH:O	2.11	0.51
1:D:576:GLU:O	1:D:579:ARG:HB2	2.10	0.51
1:D:717:ALA:O	1:D:723:ILE:HA	2.10	0.51
1:E:744:VAL:CG2	1:E:770:ILE:HG22	2.39	0.51
1:F:634:ARG:HH21	1:F:643:GLU:HB3	1.74	0.51
1:D:631:PRO:HD2	1:D:635:TRP:CZ2	2.45	0.51
1:A:274:THR:HG22	1:A:275:THR:N	2.26	0.51
1:B:463:LEU:O	1:B:477:VAL:HG22	2.10	0.51
1:E:18:HIS:O	1:E:38:PRO:HA	2.10	0.51
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.92	0.51
1:D:300:LEU:CD1	1:D:340:LEU:HD21	2.39	0.51
1:D:544:SER:HG	1:D:546:ARG:HH12	1.57	0.51
1:C:634:ARG:HG2	1:C:692:ASN:OD1	2.10	0.51
1:D:313:PHE:HA	1:D:381:GLN:HE22	1.76	0.51
1:F:201:MET:HE3	1:F:502:LEU:HD23	1.92	0.51
1:A:735:THR:HG23	1:A:760:VAL:CG1	2.41	0.50
1:B:690:LEU:HD11	1:B:693:LEU:HG	1.93	0.50
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.40	0.50
1:A:576:GLU:HG3	1:A:611:GLY:HA3	1.92	0.50
1:C:18:HIS:O	1:C:38:PRO:HA	2.12	0.50
1:A:201:MET:HE1	1:A:247:PRO:CB	2.34	0.50
1:E:289:PHE:CZ	1:E:545:TYR:CD1	3.00	0.50
1:B:606:ARG:NH1	5:B:3101:HOH:O	2.41	0.50
1:F:267:TRP:CE3	1:F:341:LYS:HG3	2.47	0.50
1:B:689:HIS:CG	1:B:739:ARG:HH11	2.29	0.50
1:F:32:MET:HE2	1:F:94:ILE:HG23	1.93	0.50
1:B:619:VAL:HG11	1:B:624:GLY:HA2	1.93	0.50
1:D:381:GLN:CB	1:D:384:LEU:HD12	2.34	0.49
1:B:329:GLU:O	1:B:332:ILE:HG13	2.11	0.49
1:E:747:LEU:HD11	1:E:752:GLN:HB3	1.94	0.49
1:D:353:LYS:HG2	1:D:353:LYS:O	2.11	0.49
1:C:275:THR:CG2	1:C:281:TYR:CZ	2.95	0.49
1:C:630:LEU:O	1:C:647:SER:N	2.45	0.49
1:C:425:VAL:CG2	1:C:426:GLN:H	2.24	0.49
1:E:32:MET:HE3	1:E:94:ILE:HG23	1.93	0.49
1:F:766:ASN:HD22	1:F:767:ALA:N	2.10	0.49
1:F:367:LEU:HG	1:F:425:VAL:CG2	2.43	0.49
1:B:474:LYS:O	1:B:476:PRO:HD3	2.12	0.49
1:F:267:TRP:CD2	1:F:341:LYS:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:LEU:O	1:A:647:SER:N	2.44	0.49
1:E:526:ARG:HD2	1:E:619:VAL:HB	1.94	0.49
1:B:273:LEU:HD22	1:B:274:THR:H	1.76	0.48
1:C:160:GLU:HA	1:C:203:ASN:OD1	2.13	0.48
1:D:120:LEU:HB3	1:D:132:SER:HB3	1.95	0.48
1:B:738:LEU:HD11	1:B:770:ILE:HG21	1.95	0.48
1:C:515:PHE:HD1	1:C:516:GLU:HG2	1.78	0.48
1:C:20:LEU:HD22	1:C:134:VAL:CG2	2.43	0.48
1:F:501:GLY:HA3	5:F:3119:HOH:O	2.14	0.48
1:A:744:VAL:HG22	1:A:746:GLY:H	1.78	0.48
1:B:18:HIS:O	1:B:38:PRO:HA	2.14	0.48
1:B:167:GLU:HB3	1:B:195:LYS:HB2	1.96	0.48
1:C:31:GLU:OE1	1:C:56:ARG:HD3	2.14	0.48
1:D:349:TYR:HB3	1:D:384:LEU:HD21	1.95	0.48
1:B:347:ASN:HB2	1:B:348:PRO:CD	2.44	0.48
1:C:692:ASN:N	1:C:692:ASN:HD22	2.11	0.48
1:D:219:GLU:HB2	1:D:229:GLN:HB3	1.96	0.47
1:C:275:THR:CG2	1:C:276:SER:O	2.62	0.47
1:A:748:GLN:CG	1:A:769:THR:HG23	2.43	0.47
1:E:134:VAL:O	1:E:135:LYS:HB2	2.14	0.47
1:A:619:VAL:HG11	1:A:624:GLY:HA2	1.97	0.47
1:D:183:ASN:HB3	1:D:419:GLU:HB3	1.96	0.47
1:D:174:ARG:NH2	5:D:3028:HOH:O	2.31	0.47
1:B:275:THR:O	1:B:276:SER:HB2	2.13	0.47
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.62	0.47
1:D:346:ILE:HD11	1:D:415:THR:HG22	1.95	0.47
1:A:679:ASP:OD1	1:A:679:ASP:N	2.47	0.47
1:B:332:ILE:HD13	1:B:409:GLY:HA3	1.96	0.47
1:B:348:PRO:HG3	1:B:444:TYR:CE1	2.50	0.47
1:F:761:VAL:CG1	1:F:768:LEU:HD11	2.44	0.47
1:F:368:LYS:O	1:F:425:VAL:HG22	2.15	0.47
1:A:522:HIS:CG	1:A:622:GLU:HG3	2.49	0.47
1:A:484:TYR:O	1:A:489:SER:HB3	2.14	0.47
1:B:20:LEU:HD22	1:B:134:VAL:HG22	1.96	0.47
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.50	0.47
1:F:367:LEU:HG	1:F:425:VAL:HG21	1.95	0.47
1:C:560:ARG:CG	1:C:560:ARG:HH11	2.26	0.47
1:F:631:PRO:HD2	1:F:635:TRP:CZ2	2.50	0.47
1:C:274:THR:HG21	1:C:540:HIS:CG	2.50	0.46
1:C:104:LYS:HG3	1:C:109:SER:HB3	1.98	0.46
1:C:744:VAL:HG22	1:C:746:GLY:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.15	0.46
1:C:560:ARG:NH1	1:C:560:ARG:HG3	2.29	0.46
1:F:485:ALA:HB1	1:F:519:ALA:HB2	1.97	0.46
1:D:540:HIS:CG	1:D:541:GLY:N	2.82	0.46
1:E:356:VAL:CG1	1:E:397:TRP:HZ2	2.27	0.46
1:D:84:LEU:HG	1:D:257:PHE:CZ	2.51	0.46
1:D:95:GLU:HG2	1:D:97:THR:HG23	1.96	0.46
1:C:516:GLU:O	1:C:517:ASN:HB2	2.15	0.46
1:A:100:TYR:CG	1:A:111:ARG:HD2	2.50	0.46
1:C:300:LEU:CD1	1:C:340:LEU:HD21	2.46	0.46
1:D:275:THR:O	1:D:276:SER:CB	2.60	0.46
1:A:70:GLU:HG3	5:A:3182:HOH:O	2.15	0.46
1:F:300:LEU:CD1	1:F:340:LEU:HD21	2.45	0.46
1:E:165:LEU:HA	1:E:197:ILE:O	2.15	0.46
1:A:725:VAL:HB	1:A:768:LEU:HB3	1.97	0.46
1:C:617:ALA:O	1:C:660:PRO:HD2	2.16	0.46
1:B:130:THR:OG1	1:B:131:GLY:N	2.48	0.46
1:C:300:LEU:HD13	1:C:340:LEU:CD2	2.46	0.46
1:A:336:LYS:HG3	1:A:342:ILE:HD13	1.98	0.46
1:E:267:TRP:CD2	1:E:341:LYS:HG3	2.51	0.46
1:D:668:LEU:O	1:D:701:CYS:HB2	2.15	0.46
1:B:20:LEU:HD22	1:B:134:VAL:CG2	2.45	0.45
1:C:646:GLY:O	1:C:647:SER:HB3	2.16	0.45
1:B:290:ILE:CD1	1:B:335:LEU:HD22	2.46	0.45
1:D:747:LEU:HD13	1:D:750:GLY:O	2.15	0.45
1:E:274:THR:HB	1:E:539:LEU:O	2.16	0.45
1:F:684:GLU:HG2	1:F:732:LYS:HB2	1.99	0.45
1:A:690:LEU:HD11	1:A:693:LEU:HG	1.98	0.45
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.17	0.45
1:D:588:MET:HG3	1:D:608:TYR:CD1	2.51	0.45
1:D:684:GLU:HG2	1:D:732:LYS:HB2	1.98	0.45
1:F:766:ASN:HD22	1:F:767:ALA:H	1.64	0.45
1:A:453:LYS:HG3	1:A:458:GLU:HG3	1.97	0.45
1:F:219:GLU:HB2	1:F:229:GLN:HB3	1.98	0.45
1:A:308:PHE:CZ	1:B:44:ARG:HB3	2.52	0.45
1:E:201:MET:CE	1:E:247:PRO:HB3	2.47	0.45
1:D:267:TRP:HA	1:D:678:PRO:HG2	1.98	0.45
1:B:274:THR:HB	1:B:539:LEU:O	2.17	0.45
1:D:315:TRP:CE3	1:D:381:GLN:OE1	2.70	0.45
1:A:744:VAL:HG23	1:A:770:ILE:HD12	1.98	0.45
1:A:681:VAL:HG22	1:A:684:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:HD3	1:A:243:ASP:OD1	2.17	0.45
1:A:367:LEU:HD11	1:A:425:VAL:HG13	1.97	0.45
1:F:579:ARG:HD2	1:F:589:ARG:HH22	1.82	0.45
1:F:748:GLN:HG3	1:F:769:THR:HB	1.98	0.45
1:D:483:CYS:SG	1:D:514:GLY:HA2	2.57	0.45
1:B:327:ASP:OD2	1:B:330:GLY:HA3	2.16	0.45
1:B:315:TRP:O	1:B:350:ILE:HA	2.16	0.45
1:D:184:ARG:HD3	1:D:192:GLN:CD	2.37	0.45
1:D:274:THR:HG23	1:D:304:HIS:CD2	2.47	0.45
1:F:681:VAL:HG23	1:F:683:HIS:CE1	2.52	0.45
1:F:417:PHE:HA	1:F:419:GLU:OE2	2.16	0.45
1:B:183:ASN:HA	1:B:196:ASN:ND2	2.32	0.45
1:E:548:PRO:HB2	1:E:556:CYS:SG	2.57	0.45
1:B:369:ARG:HB3	1:B:370:PRO:HD2	1.99	0.44
1:B:165:LEU:HA	1:B:197:ILE:O	2.16	0.44
1:F:694:GLN:O	1:F:697:HIS:HB2	2.17	0.44
1:F:290:ILE:HD11	1:F:335:LEU:HD22	1.95	0.44
1:E:533:LEU:HD21	1:E:569:MET:CE	2.47	0.44
1:C:598:ASP:HA	1:C:599:PRO:HD2	1.87	0.44
1:C:17:ILE:HG13	1:C:139:TYR:HB3	1.99	0.44
1:F:152:GLU:HB3	1:F:230:PHE:CE1	2.52	0.44
1:F:201:MET:HE3	1:F:502:LEU:CD2	2.47	0.44
1:E:515:PHE:CD1	1:E:516:GLU:HG2	2.52	0.44
1:F:763:PRO:HB3	1:F:768:LEU:HD22	1.98	0.44
1:B:414:LYS:NZ	1:B:538:ARG:HH12	2.13	0.44
1:C:195:LYS:HB3	1:C:468:ALA:HB3	2.00	0.44
1:F:167:GLU:OE2	1:F:195:LYS:NZ	2.36	0.44
1:D:727:GLY:H	1:D:766:ASN:ND2	2.08	0.44
1:E:340:LEU:HA	1:E:340:LEU:HD23	1.84	0.44
1:C:174:ARG:HB3	1:C:220:VAL:HG11	1.99	0.44
1:B:219:GLU:HB2	1:B:229:GLN:HB3	2.00	0.44
1:B:725:VAL:HB	1:B:768:LEU:HB3	1.99	0.44
1:F:201:MET:CE	1:F:502:LEU:CD2	2.95	0.44
1:E:32:MET:CE	1:E:94:ILE:HG23	2.47	0.44
1:F:744:VAL:CG2	1:F:770:ILE:HD12	2.48	0.44
1:D:695:ASP:HA	1:D:718:ARG:HD3	2.00	0.44
1:E:324:THR:CG2	1:E:325:PHE:CD2	2.99	0.44
1:C:684:GLU:HG2	1:C:732:LYS:HB2	2.00	0.44
1:F:333:ARG:NH1	2:F:3009:SO4:O4	2.29	0.44
1:F:333:ARG:NH1	2:F:3009:SO4:S	2.90	0.44
1:D:196:ASN:O	1:D:197:ILE:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:416:ASP:OD1	1:E:466:ARG:HD3	2.18	0.44
1:E:723:ILE:HG12	1:E:770:ILE:HB	1.99	0.44
1:E:109:SER:O	1:E:122:PHE:HA	2.18	0.44
1:C:61:GLN:HB2	1:C:64:ILE:HD12	2.00	0.44
1:B:32:MET:CE	1:B:102:GLU:O	2.66	0.44
1:F:297:ASN:O	1:F:560:ARG:HD3	2.17	0.44
1:C:11:GLN:HA	1:C:12:PRO:HD3	1.83	0.44
1:D:17:ILE:HG13	1:D:139:TYR:HB3	2.00	0.44
1:A:770:ILE:O	1:A:770:ILE:HG13	2.16	0.43
1:F:744:VAL:HG22	1:F:746:GLY:H	1.82	0.43
1:B:629:TYR:HA	1:B:649:TRP:HA	2.00	0.43
1:D:277:PHE:CD2	1:D:278:THR:HG23	2.52	0.43
1:B:32:MET:HE1	1:B:102:GLU:O	2.18	0.43
1:C:306:ASP:O	1:C:309:TRP:HD1	2.01	0.43
1:C:588:MET:HG3	1:C:608:TYR:CD1	2.53	0.43
1:D:541:GLY:HA3	1:D:546:ARG:CZ	2.49	0.43
1:A:554:GLU:O	1:A:558:VAL:HG23	2.19	0.43
1:F:300:LEU:HD13	1:F:340:LEU:HD21	2.00	0.43
1:D:515:PHE:HB3	1:D:516:GLU:H	1.69	0.43
1:A:321:ASP:HA	1:A:322:PRO:HD3	1.86	0.43
1:F:735:THR:HG23	1:F:760:VAL:CG1	2.48	0.43
1:B:347:ASN:CB	1:B:348:PRO:CD	2.97	0.43
1:D:165:LEU:HA	1:D:197:ILE:O	2.18	0.43
1:E:191:GLU:N	1:E:191:GLU:OE1	2.48	0.43
1:A:634:ARG:HD2	1:A:692:ASN:OD1	2.18	0.43
1:C:619:VAL:HG11	1:C:624:GLY:HA2	2.01	0.43
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.53	0.43
1:D:280:ASN:O	1:D:281:TYR:HB3	2.18	0.43
1:F:123:LEU:HD22	1:F:123:LEU:N	2.33	0.43
1:D:381:GLN:HE21	1:D:381:GLN:HA	1.83	0.43
1:E:136:ASN:HD21	1:E:227:LYS:HE3	1.83	0.43
1:B:447:LEU:C	1:B:447:LEU:HD23	2.38	0.43
1:E:689:HIS:ND1	1:E:739:ARG:HD3	2.33	0.43
1:F:664:ARG:HD2	1:F:664:ARG:HH11	1.67	0.43
1:B:715:LYS:O	1:B:725:VAL:HA	2.19	0.43
1:C:174:ARG:O	1:C:177:GLN:HG2	2.19	0.43
1:F:61:GLN:HB2	1:F:64:ILE:HD12	1.99	0.43
1:A:747:LEU:HD13	1:A:750:GLY:O	2.18	0.43
1:C:764:GLN:HG2	1:C:764:GLN:O	2.19	0.43
1:F:346:ILE:HD11	1:F:415:THR:HG22	2.01	0.43
1:C:763:PRO:HB3	1:C:768:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ILE:CD1	1:D:335:LEU:HD22	2.49	0.42
1:D:595:PHE:CE1	1:D:631:PRO:HG2	2.53	0.42
1:C:692:ASN:H	1:C:692:ASN:HD22	1.65	0.42
1:A:498:LEU:HD21	1:A:608:TYR:HB3	2.01	0.42
1:F:735:THR:CG2	1:F:760:VAL:HG13	2.49	0.42
1:D:201:MET:CE	1:D:247:PRO:HB3	2.49	0.42
1:B:613:ASN:HA	1:B:664:ARG:HD2	2.00	0.42
1:C:55:LEU:HD12	1:C:55:LEU:N	2.33	0.42
1:F:18:HIS:O	1:F:38:PRO:HA	2.18	0.42
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.54	0.42
1:C:201:MET:HE1	1:C:247:PRO:HB3	2.00	0.42
1:F:668:LEU:HD21	1:F:714:LEU:HD13	2.00	0.42
1:F:396:LYS:NZ	1:F:400:ASP:OD2	2.34	0.42
1:A:448:VAL:HG12	1:A:463:LEU:HD21	2.02	0.42
1:A:261:PRO:HA	1:A:473:GLN:O	2.19	0.42
1:B:472:ALA:HB1	5:B:3089:HOH:O	2.20	0.42
1:F:300:LEU:HD13	1:F:340:LEU:CD2	2.49	0.42
1:F:261:PRO:HA	1:F:473:GLN:O	2.20	0.42
1:C:576:GLU:HG3	1:C:611:GLY:HA3	2.01	0.42
1:B:717:ALA:O	1:B:723:ILE:HA	2.19	0.42
1:C:275:THR:HG21	1:C:281:TYR:CE2	2.54	0.42
1:C:20:LEU:HD22	1:C:134:VAL:HG22	2.00	0.42
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.54	0.42
1:A:261:PRO:O	1:A:581:ASN:HA	2.20	0.42
1:A:414:LYS:NZ	1:A:538:ARG:HH12	2.17	0.42
1:C:689:HIS:CE1	1:C:739:ARG:NH1	2.87	0.42
1:C:560:ARG:CG	1:C:560:ARG:NH1	2.81	0.42
1:B:321:ASP:HA	1:B:322:PRO:HD3	1.86	0.42
1:B:429:ASP:OD1	1:B:431:SER:OG	2.36	0.42
1:C:167:GLU:HB2	1:C:500:ILE:HG13	2.01	0.42
1:D:211:ASN:ND2	1:D:238:GLU:OE1	2.48	0.42
1:B:657:LEU:HB2	5:B:3155:HOH:O	2.20	0.42
1:B:291:ASP:O	1:B:295:GLU:HG3	2.20	0.42
1:C:425:VAL:HG23	1:C:426:GLN:H	1.85	0.42
1:C:431:SER:HB3	1:C:436:MET:HG2	2.02	0.42
1:B:555:SER:O	1:B:559:VAL:HG23	2.20	0.42
1:C:715:LYS:O	1:C:725:VAL:HA	2.19	0.42
1:C:459:GLU:H	1:C:459:GLU:CD	2.22	0.42
1:C:347:ASN:CB	1:C:348:PRO:CD	2.96	0.42
1:C:744:VAL:HG22	1:C:746:GLY:N	2.35	0.42
1:F:1:MET:N	1:F:219:GLU:OE2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:GLU:HG3	1:D:204:ARG:HG2	2.02	0.42
1:B:598:ASP:HA	1:B:599:PRO:HD2	1.93	0.42
1:B:408:MET:O	1:B:408:MET:HG2	2.19	0.42
1:B:168:ARG:HG3	1:B:174:ARG:NH2	2.35	0.42
1:E:163:TYR:HB3	1:E:502:LEU:HD13	2.01	0.42
1:A:459:GLU:HG3	1:A:459:GLU:H	1.69	0.42
1:D:540:HIS:N	1:D:546:ARG:HD2	2.35	0.41
1:D:347:ASN:HA	1:D:444:TYR:OH	2.19	0.41
1:B:98:GLU:H	1:B:98:GLU:CD	2.24	0.41
1:B:123:LEU:HA	1:B:127:GLU:O	2.20	0.41
1:E:565:LEU:O	1:E:569:MET:HG3	2.20	0.41
1:D:631:PRO:O	1:D:646:GLY:HA3	2.20	0.41
1:C:767:ALA:O	1:C:768:LEU:O	2.37	0.41
1:D:725:VAL:HB	1:D:768:LEU:HD12	2.02	0.41
1:D:358:LYS:O	1:D:362:GLU:HG3	2.20	0.41
1:F:273:LEU:HD23	1:F:539:LEU:HB2	2.02	0.41
1:E:296:ARG:O	1:E:560:ARG:NH1	2.52	0.41
1:B:195:LYS:HE2	1:B:478:HIS:HB3	2.03	0.41
1:C:315:TRP:O	1:C:350:ILE:HA	2.19	0.41
1:E:315:TRP:O	1:E:350:ILE:HA	2.20	0.41
1:E:300:LEU:HD13	1:E:300:LEU:C	2.40	0.41
1:E:300:LEU:HD13	1:E:301:HIS:N	2.35	0.41
1:A:414:LYS:HE3	1:A:479:TRP:CH2	2.56	0.41
1:C:579:ARG:NH1	1:C:579:ARG:HG3	2.36	0.41
1:D:463:LEU:O	1:D:477:VAL:HG22	2.20	0.41
1:B:31:GLU:HG2	1:B:58:PHE:HB3	2.02	0.41
1:C:150:MET:HB3	1:C:237:LEU:HB2	2.01	0.41
1:F:212:HIS:HA	1:F:213:PRO:HD3	1.87	0.41
1:D:384:LEU:C	1:D:384:LEU:HD23	2.40	0.41
1:A:123:LEU:HD12	1:A:128:ARG:HA	2.02	0.41
1:F:619:VAL:HG11	1:F:624:GLY:HA2	2.01	0.41
1:C:17:ILE:CG1	1:C:139:TYR:HB3	2.51	0.41
1:E:382:PRO:HG2	5:E:3049:HOH:O	2.20	0.41
1:E:489:SER:O	1:E:492:GLU:HG2	2.20	0.41
1:C:570:MET:HG3	1:C:678:PRO:HA	2.02	0.41
1:F:579:ARG:NH1	1:F:579:ARG:HG3	2.32	0.41
1:B:150:MET:HB3	1:B:237:LEU:HB2	2.01	0.41
1:E:165:LEU:HD12	1:E:174:ARG:HG2	2.03	0.41
1:B:674:ASN:HB3	1:B:680:TYR:CE1	2.56	0.41
1:C:32:MET:HB2	1:C:94:ILE:HD13	2.02	0.41
1:E:540:HIS:C	1:E:546:ARG:HG3	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:HG12	1:B:463:LEU:HD21	2.02	0.41
1:C:170:THR:HG1	1:C:177:GLN:HE22	1.61	0.41
1:C:526:ARG:HD2	1:C:619:VAL:HB	2.02	0.41
1:B:341:LYS:O	1:B:342:ILE:HD12	2.20	0.41
1:F:31:GLU:OE1	1:F:56:ARG:HD3	2.21	0.41
1:F:617:ALA:O	1:F:660:PRO:HD2	2.21	0.41
1:A:18:HIS:O	1:A:38:PRO:HA	2.21	0.41
1:F:459:GLU:HG3	1:F:459:GLU:H	1.29	0.41
1:C:692:ASN:ND2	1:C:692:ASN:N	2.69	0.41
1:E:680:TYR:CE2	1:E:682:TRP:HD1	2.39	0.41
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.56	0.41
1:B:749:ASP:HB3	1:B:765:GLY:O	2.21	0.41
1:E:652:GLN:NE2	1:E:654:HIS:NE2	2.69	0.40
1:D:278:THR:HG21	1:E:45:THR:HA	2.03	0.40
1:F:291:ASP:OD1	1:F:338:LYS:NZ	2.54	0.40
1:C:485:ALA:HB1	1:C:519:ALA:HB2	2.03	0.40
1:F:681:VAL:HG13	1:F:684:GLU:HB2	2.02	0.40
1:D:509:SER:HB3	1:D:536:HIS:CB	2.52	0.40
1:A:622:GLU:HA	5:A:3158:HOH:O	2.22	0.40
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.66	0.40
1:A:367:LEU:HD11	1:A:425:VAL:CG1	2.51	0.40
1:E:508:TRP:CZ3	1:E:510:HIS:CD2	3.09	0.40
1:B:167:GLU:OE2	1:B:195:LYS:NZ	2.46	0.40
1:F:333:ARG:NH1	2:F:3009:SO4:O3	2.54	0.40
1:F:668:LEU:O	1:F:701:CYS:HB2	2.22	0.40
1:E:490:MET:HE2	1:E:620:PHE:CD1	2.56	0.40
1:F:320:TRP:CD2	1:F:328:PRO:HB3	2.56	0.40
1:E:212:HIS:HA	1:E:213:PRO:HD3	1.87	0.40
1:A:195:LYS:HE2	1:A:478:HIS:HB3	2.03	0.40
1:C:275:THR:HG23	1:C:281:TYR:CZ	2.56	0.40
1:F:767:ALA:O	1:F:769:THR:N	2.55	0.40
1:F:199:PHE:HA	1:F:208:VAL:O	2.20	0.40
1:C:713:THR:O	1:C:727:GLY:HA2	2.21	0.40
1:D:526:ARG:HD2	1:D:619:VAL:HB	2.03	0.40
1:E:274:THR:CG2	1:E:540:HIS:ND1	2.60	0.40
1:E:38:PRO:HG2	1:E:51:PRO:HD2	2.03	0.40
1:D:525:LYS:HG2	1:D:558:VAL:HG21	2.03	0.40
1:E:747:LEU:HD12	1:E:752:GLN:HE21	1.85	0.40
1:F:634:ARG:HH21	1:F:643:GLU:CB	2.35	0.40
1:C:84:LEU:HD12	1:C:258:THR:HG22	2.04	0.40
1:E:588:MET:HG3	1:E:608:TYR:CD1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:LYS:HE3	1:F:453:LYS:HB3	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	771/778 (99%)	744 (96%)	25 (3%)	2 (0%)	46	50
1	B	771/778 (99%)	731 (95%)	37 (5%)	3 (0%)	39	42
1	C	771/778 (99%)	740 (96%)	27 (4%)	4 (0%)	34	35
1	D	771/778 (99%)	733 (95%)	32 (4%)	6 (1%)	24	22
1	E	771/778 (99%)	738 (96%)	29 (4%)	4 (0%)	34	35
1	F	771/778 (99%)	739 (96%)	26 (3%)	6 (1%)	24	22
All	All	4626/4668 (99%)	4425 (96%)	176 (4%)	25 (0%)	34	35

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	768	LEU
1	B	767	ALA
1	C	766	ASN
1	C	768	LEU
1	E	768	LEU
1	F	767	ALA
1	B	768	LEU
1	C	477	VAL
1	C	767	ALA
1	D	276	SER
1	D	316	CYS

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Mol	Chain	Res	Type
1	D	477	VAL
1	F	768	LEU
1	F	316	CYS
1	D	720	GLY
1	B	477	VAL
1	E	477	VAL
1	F	477	VAL
1	F	720	GLY
1	A	348	PRO
1	D	515	PHE
1	E	47	GLN
1	F	766	ASN
1	D	348	PRO
1	E	720	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	659/665 (99%)	613 (93%)	46 (7%)	19	19
1	B	659/665 (99%)	613 (93%)	46 (7%)	19	19
1	C	659/665 (99%)	615 (93%)	44 (7%)	20	21
1	D	659/665 (99%)	608 (92%)	51 (8%)	16	16
1	E	659/665 (99%)	603 (92%)	56 (8%)	13	13
1	F	659/665 (99%)	608 (92%)	51 (8%)	16	16
All	All	3954/3990 (99%)	3660 (93%)	294 (7%)	17	17

All (294) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	44	ARG
1	A	48	LEU
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	69	ILE
1	A	84	LEU
1	A	91	LYS
1	A	99	ARG
1	A	116	GLU
1	A	120	LEU
1	A	123	LEU
1	A	128	ARG
1	A	174	ARG
1	A	179	VAL
1	A	208	VAL
1	A	300	LEU
1	A	311	LYS
1	A	336	LYS
1	A	377	TRP
1	A	419	GLU
1	A	425	VAL
1	A	431	SER
1	A	452	LEU
1	A	459	GLU
1	A	464	PHE
1	A	479	TRP
1	A	492	GLU
1	A	533	LEU
1	A	573	LEU
1	A	592	MET
1	A	630	LEU
1	A	657	LEU
1	A	671	LEU
1	A	681	VAL
1	A	693	LEU
1	A	714	LEU
1	A	723	ILE
1	A	732	LYS
1	A	735	THR
1	A	736	LEU
1	A	748	GLN
1	A	764	GLN
1	A	766	ASN
1	A	768	LEU
1	A	769	THR
1	A	770	ILE

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Mol	Chain	Res	Type
1	B	52	LEU
1	B	69	ILE
1	B	84	LEU
1	B	99	ARG
1	B	120	LEU
1	B	123	LEU
1	B	143	THR
1	B	177	GLN
1	B	204	ARG
1	B	208	VAL
1	B	227	LYS
1	B	273	LEU
1	B	274	THR
1	B	285	THR
1	B	316	CYS
1	B	329	GLU
1	B	338	LYS
1	B	342	ILE
1	B	377	TRP
1	B	452	LEU
1	B	459	GLU
1	B	464	PHE
1	B	479	TRP
1	B	533	LEU
1	B	573	LEU
1	B	592	MET
1	B	616	VAL
1	B	625	ASP
1	B	630	LEU
1	B	634	ARG
1	B	653	GLN
1	B	657	LEU
1	B	664	ARG
1	B	671	LEU
1	B	693	LEU
1	B	714	LEU
1	B	719	THR
1	B	726	THR
1	B	732	LYS
1	B	739	ARG
1	B	744	VAL
1	B	747	LEU

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Mol	Chain	Res	Type
1	B	748	GLN
1	B	764	GLN
1	B	768	LEU
1	B	771	THR
1	C	20	LEU
1	C	38	PRO
1	C	48	LEU
1	C	52	LEU
1	C	84	LEU
1	C	120	LEU
1	C	146	GLN
1	C	174	ARG
1	C	204	ARG
1	C	273	LEU
1	C	275	THR
1	C	300	LEU
1	C	306	ASP
1	C	316	CYS
1	C	348	PRO
1	C	350	ILE
1	C	377	TRP
1	C	408	MET
1	C	419	GLU
1	C	452	LEU
1	C	459	GLU
1	C	464	PHE
1	C	477	VAL
1	C	479	TRP
1	C	500	ILE
1	C	533	LEU
1	C	553	ASP
1	C	573	LEU
1	C	579	ARG
1	C	614	VAL
1	C	616	VAL
1	C	630	LEU
1	C	657	LEU
1	C	671	LEU
1	C	693	LEU
1	C	714	LEU
1	C	735	THR
1	C	736	LEU

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Mol	Chain	Res	Type
1	C	739	ARG
1	C	747	LEU
1	C	764	GLN
1	C	768	LEU
1	C	770	ILE
1	C	772	LEU
1	D	48	LEU
1	D	52	LEU
1	D	69	ILE
1	D	84	LEU
1	D	120	LEU
1	D	143	THR
1	D	174	ARG
1	D	177	GLN
1	D	178	THR
1	D	208	VAL
1	D	273	LEU
1	D	289	PHE
1	D	300	LEU
1	D	306	ASP
1	D	316	CYS
1	D	333	ARG
1	D	336	LYS
1	D	342	ILE
1	D	377	TRP
1	D	419	GLU
1	D	452	LEU
1	D	459	GLU
1	D	477	VAL
1	D	517	ASN
1	D	525	LYS
1	D	533	LEU
1	D	540	HIS
1	D	543	LYS
1	D	545	TYR
1	D	546	ARG
1	D	573	LEU
1	D	592	MET
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	671	LEU

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Mol	Chain	Res	Type
1	D	693	LEU
1	D	714	LEU
1	D	719	THR
1	D	723	ILE
1	D	726	THR
1	D	735	THR
1	D	736	LEU
1	D	742	VAL
1	D	744	VAL
1	D	745	ASN
1	D	747	LEU
1	D	748	GLN
1	D	764	GLN
1	D	771	THR
1	D	772	LEU
1	E	20	LEU
1	E	44	ARG
1	E	45	THR
1	E	47	GLN
1	E	48	LEU
1	E	84	LEU
1	E	98	GLU
1	E	116	GLU
1	E	120	LEU
1	E	127	GLU
1	E	128	ARG
1	E	143	THR
1	E	146	GLN
1	E	174	ARG
1	E	177	GLN
1	E	178	THR
1	E	179	VAL
1	E	195	LYS
1	E	204	ARG
1	E	208	VAL
1	E	214	GLN
1	E	274	THR
1	E	288	SER
1	E	311	LYS
1	E	316	CYS
1	E	324	THR
1	E	377	TRP

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Mol	Chain	Res	Type
1	E	419	GLU
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	477	VAL
1	E	479	TRP
1	E	573	LEU
1	E	592	MET
1	E	614	VAL
1	E	616	VAL
1	E	625	ASP
1	E	630	LEU
1	E	632	GLU
1	E	653	GLN
1	E	681	VAL
1	E	693	LEU
1	E	719	THR
1	E	723	ILE
1	E	726	THR
1	E	735	THR
1	E	736	LEU
1	E	742	VAL
1	E	744	VAL
1	E	747	LEU
1	E	748	GLN
1	E	757	GLN
1	E	764	GLN
1	E	769	THR
1	E	772	LEU
1	F	27	GLN
1	F	39	ARG
1	F	52	LEU
1	F	69	ILE
1	F	84	LEU
1	F	120	LEU
1	F	127	GLU
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	204	ARG
1	F	273	LEU
1	F	280	ASN

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Mol	Chain	Res	Type
1	F	300	LEU
1	F	316	CYS
1	F	377	TRP
1	F	408	MET
1	F	419	GLU
1	F	425	VAL
1	F	452	LEU
1	F	453	LYS
1	F	459	GLU
1	F	464	PHE
1	F	477	VAL
1	F	479	TRP
1	F	518	THR
1	F	533	LEU
1	F	573	LEU
1	F	592	MET
1	F	614	VAL
1	F	616	VAL
1	F	630	LEU
1	F	632	GLU
1	F	657	LEU
1	F	671	LEU
1	F	693	LEU
1	F	714	LEU
1	F	719	THR
1	F	726	THR
1	F	732	LYS
1	F	735	THR
1	F	736	LEU
1	F	739	ARG
1	F	742	VAL
1	F	747	LEU
1	F	748	GLN
1	F	756	GLU
1	F	764	GLN
1	F	766	ASN
1	F	770	ILE
1	F	771	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	133	GLN
1	A	212	HIS
1	A	287	ASN
1	A	517	ASN
1	A	692	ASN
1	B	27	GLN
1	B	73	GLN
1	B	107	ASN
1	B	125	ASN
1	B	177	GLN
1	B	517	ASN
1	B	652	GLN
1	B	764	GLN
1	C	27	GLN
1	C	77	ASN
1	C	133	GLN
1	C	146	GLN
1	C	177	GLN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN
1	C	692	ASN
1	C	697	HIS
1	C	764	GLN
1	D	73	GLN
1	D	107	ASN
1	D	125	ASN
1	D	177	GLN
1	D	381	GLN
1	D	564	GLN
1	D	652	GLN
1	D	745	ASN
1	D	766	ASN
1	E	27	GLN
1	E	73	GLN
1	E	77	ASN
1	E	517	ASN
1	E	652	GLN
1	E	697	HIS
1	E	766	ASN
1	F	27	GLN
1	F	73	GLN

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Mol	Chain	Res	Type
1	F	77	ASN
1	F	177	GLN
1	F	517	ASN
1	F	564	GLN
1	F	627	GLN
1	F	652	GLN
1	F	692	ASN
1	F	745	ASN
1	F	752	GLN
1	F	766	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACY	A	2003	-	1,3,3	2.74	1 (100%)	0,3,3	0.00	-
2	SO4	A	3014	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	A	3017	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	A	3018	-	4,4,4	0.04	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MPO	B	1001	-	12,13,13	1.03	0	15,17,17	1.99	3 (20%)
2	SO4	B	3008	-	4,4,4	0.26	0	6,6,6	0.41	0
2	SO4	B	3010	-	4,4,4	0.14	0	6,6,6	0.30	0
2	SO4	B	3013	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	B	3015	-	4,4,4	0.19	0	6,6,6	0.24	0
2	SO4	B	3016	-	4,4,4	0.26	0	6,6,6	0.29	0
3	MPO	C	1002	-	12,13,13	0.92	1 (8%)	15,17,17	1.31	3 (20%)
2	SO4	C	3007	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	C	3012	-	4,4,4	0.22	0	6,6,6	0.56	0
3	MPO	D	1003	-	12,13,13	0.82	0	15,17,17	1.75	4 (26%)
2	SO4	D	3004	-	4,4,4	0.23	0	6,6,6	0.38	0
2	SO4	D	3011	-	4,4,4	0.07	0	6,6,6	0.38	0
3	MPO	E	1004	-	12,13,13	1.38	1 (8%)	15,17,17	1.42	1 (6%)
4	ACY	E	2001	-	1,3,3	1.65	0	0,3,3	0.00	-
2	SO4	E	3006	-	4,4,4	0.12	0	6,6,6	0.46	0
4	ACY	F	2002	-	1,3,3	2.11	1 (100%)	0,3,3	0.00	-
2	SO4	F	3001	-	4,4,4	0.31	0	6,6,6	0.19	0
2	SO4	F	3002	-	4,4,4	0.17	0	6,6,6	0.33	0
2	SO4	F	3003	-	4,4,4	0.22	0	6,6,6	0.60	0
2	SO4	F	3005	-	4,4,4	0.57	0	6,6,6	1.04	0
2	SO4	F	3009	-	4,4,4	0.26	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACY	A	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3014	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3017	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3018	-	-	0/0/0/0	0/0/0/0
3	MPO	B	1001	-	-	0/7/15/15	0/1/1/1
2	SO4	B	3008	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3010	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3013	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3015	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3016	-	-	0/0/0/0	0/0/0/0
3	MPO	C	1002	-	-	0/7/15/15	0/1/1/1
2	SO4	C	3007	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3012	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPO	D	1003	-	-	0/7/15/15	0/1/1/1
2	SO4	D	3004	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3011	-	-	0/0/0/0	0/0/0/0
3	MPO	E	1004	-	-	0/7/15/15	0/1/1/1
4	ACY	E	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	E	3006	-	-	0/0/0/0	0/0/0/0
4	ACY	F	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3001	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3002	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3003	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3005	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3009	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	MPO	O3-S1	2.03	1.51	1.46
4	F	2002	ACY	CH3-C	2.11	1.51	1.48
3	E	1004	MPO	O3-S1	2.69	1.53	1.46
4	A	2003	ACY	CH3-C	2.74	1.52	1.48

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1003	MPO	O4-C6-C7	-2.94	105.10	111.84
3	C	1002	MPO	C5-C4-N1	-2.27	106.69	110.12
3	C	1002	MPO	C3-N1-C7	-2.19	105.65	111.27
3	B	1001	MPO	O4-C5-C4	-2.08	107.07	111.84
3	C	1002	MPO	O2-S1-C1	2.01	108.62	106.91
3	D	1003	MPO	O1-S1-C1	2.16	108.75	106.91
3	D	1003	MPO	C7-N1-C4	2.33	113.95	108.90
3	B	1001	MPO	O2-S1-C1	2.94	109.42	106.91
3	D	1003	MPO	O2-S1-C1	3.79	110.14	106.91
3	E	1004	MPO	O2-S1-C1	4.01	110.33	106.91
3	B	1001	MPO	O1-S1-C1	5.37	111.49	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3006	SO4	1	0
2	F	3005	SO4	1	0
2	F	3009	SO4	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	773/778 (99%)	-0.36	4 (0%) 91 91	18, 29, 47, 71	0
1	B	773/778 (99%)	-0.01	26 (3%) 49 47	23, 36, 60, 81	0
1	C	773/778 (99%)	-0.26	3 (0%) 93 93	20, 30, 47, 75	0
1	D	773/778 (99%)	-0.13	19 (2%) 61 60	19, 32, 64, 78	0
1	E	773/778 (99%)	-0.20	6 (0%) 87 87	20, 33, 57, 89	0
1	F	773/778 (99%)	-0.33	5 (0%) 90 90	21, 31, 50, 69	0
All	All	4638/4668 (99%)	-0.22	63 (1%) 78 77	18, 32, 55, 89	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	765	GLY	6.6
1	D	278	THR	6.5
1	B	767	ALA	6.0
1	D	275	THR	5.4
1	D	545	TYR	5.4
1	C	765	GLY	5.4
1	B	766	ASN	5.1
1	D	277	PHE	4.9
1	B	768	LEU	4.8
1	D	765	GLY	4.8
1	F	768	LEU	4.7
1	D	541	GLY	4.4
1	F	719	THR	4.2
1	E	765	GLY	4.1
1	E	766	ASN	4.0
1	A	768	LEU	3.8
1	B	764	GLN	3.8
1	D	540	HIS	3.8
1	B	407	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	719	THR	3.7
1	E	43	GLU	3.6
1	A	765	GLY	3.6
1	C	767	ALA	3.5
1	F	766	ASN	3.3
1	D	281	TYR	3.0
1	D	546	ARG	3.0
1	D	279	THR	2.9
1	B	337	ALA	2.8
1	D	768	LEU	2.8
1	B	744	VAL	2.8
1	B	339	GLY	2.8
1	B	745	ASN	2.8
1	D	381	GLN	2.7
1	A	766	ASN	2.7
1	B	738	LEU	2.6
1	B	743	LYS	2.6
1	B	29	ASP	2.6
1	D	766	ASN	2.5
1	B	741	VAL	2.5
1	E	745	ASN	2.5
1	B	722	THR	2.5
1	B	723	ILE	2.4
1	D	542	SER	2.4
1	D	289	PHE	2.3
1	E	40	ASP	2.3
1	F	88	GLN	2.3
1	D	380	TRP	2.3
1	B	294	ALA	2.3
1	E	98	GLU	2.3
1	B	290	ILE	2.3
1	D	747	LEU	2.3
1	B	681	VAL	2.2
1	D	276	SER	2.2
1	B	325	PHE	2.2
1	B	728	ALA	2.2
1	B	719	THR	2.1
1	B	338	LYS	2.1
1	C	766	ASN	2.1
1	D	282	ASP	2.1
1	B	545	TYR	2.1
1	B	690	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	762	LYS	2.0
1	B	305	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	3016	5/5	0.88	0.19	7.55	72,72,73,75	0
2	SO4	C	3012	5/5	0.87	0.16	4.67	66,66,69,70	0
4	ACY	F	2002	4/4	0.83	0.15	3.72	46,46,47,48	0
4	ACY	E	2001	4/4	0.85	0.16	2.90	38,39,41,41	0
4	ACY	A	2003	4/4	0.82	0.14	2.76	40,40,42,42	0
3	MPO	E	1004	13/13	0.94	0.13	0.74	51,53,58,58	0
2	SO4	F	3005	5/5	0.90	0.16	0.62	50,53,56,56	0
3	MPO	D	1003	13/13	0.96	0.14	0.50	43,52,58,58	0
3	MPO	C	1002	13/13	0.96	0.12	0.35	43,48,53,55	0
3	MPO	B	1001	13/13	0.91	0.13	-0.51	46,54,64,66	0
2	SO4	E	3006	5/5	0.96	0.15	-	56,58,59,62	0
2	SO4	A	3017	5/5	0.92	0.28	-	73,75,77,78	0
2	SO4	F	3009	5/5	0.85	0.21	-	64,66,68,69	0
2	SO4	A	3014	5/5	0.90	0.16	-	78,79,80,82	0
2	SO4	F	3002	5/5	0.96	0.17	-	60,63,65,66	0
2	SO4	D	3011	5/5	0.89	0.23	-	86,87,88,88	0
2	SO4	B	3008	5/5	0.95	0.26	-	59,61,62,63	0
2	SO4	A	3018	5/5	0.88	0.21	-	84,85,85,86	0
2	SO4	F	3001	5/5	0.89	0.13	-	65,66,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	3010	5/5	0.92	0.20	-	76,77,77,78	0
2	SO4	B	3015	5/5	0.86	0.27	-	79,81,82,82	0
2	SO4	C	3007	5/5	0.98	0.18	-	61,62,63,63	0
2	SO4	D	3004	5/5	0.96	0.15	-	65,65,66,67	0
2	SO4	F	3003	5/5	0.95	0.23	-	57,57,59,60	0
2	SO4	B	3013	5/5	0.90	0.24	-	77,78,79,80	0

6.5 Other polymers

There are no such residues in this entry.